

Robustness of Gapless Interface State in a Junction of Two Topological Insulators

Tetsuro Habe¹ and Yasuhiro Asano^{1,2}

¹*Department of Applied Physics, Hokkaido University, Sapporo 060-8628, Japan and*

²*Center for Topological Science & Technology, Hokkaido University, Sapporo 060-8628, Japan*

(Dated: February 21, 2013)

We theoretically study subgap states appearing at the interface between two three-dimensional topological insulators which have different configurations in the spin-orbit interactions from each other. The coupling of spin σ with momenta \mathbf{p} is configured by a material dependent 3×3 matrix $\mathbf{\Lambda}$ as $\sigma^\mu \Lambda_\mu^\nu p_\nu$. We show that the spectra of the interface subgap states depend strongly on the relative choices of $\mathbf{\Lambda}$ in the two topological insulators. In particular, we focus on properties of gapless states which appear when $\mathbf{\Lambda}$ in two topological insulators are connected by the inversion in momentum space. We also discuss the robustness of the gapless states under perturbations breaking the time-reversal symmetry or the band-inversion symmetry by the numerical simulation.

PACS numbers: 73.20.At, 74.45.+c

I. INTRODUCTION

Topological insulators (TIs) are new class of condensed matter¹⁻⁴. A topological number Z_2 defined in terms of the global property of wave function for the occupied states below the gap distinguishes the topological insulating phase $Z_2 = 1$ from the conventional one $Z_2 = 0$. The bulk-edge correspondence guarantees the presence of gapless states at the surface of TI^{1,3,5,6}. On the surface of three-dimensional TIs, the excitation spectra of the gapless state are described by so called Dirac cone, (i.e., $E = \pm v|\mathbf{k}|$). The strong spin-orbit interaction locks the direction of momenta and that of spin, and is responsible for the non-trivial Z_2 topological number.

When we focus on the surface state of a single TI, the spectra of the surface state are independent of the configurations in the momentum-spin locking. On the other hand, when we focus on the interface states between two different topological insulators, the spectra of the interface state depend on the relative configuration of the spin-orbit coupling in the two TIs^{7,8}. The investigation in this direction has been also done in superconducting junctions consisting of two helical superconductors⁹ and of two chiral superconductors^{10,11}. These studies focus on the discrete degree of freedom such as helicity, chirality and mirror symmetry^{12,13}. However, the coupling of spin σ with momenta \mathbf{p} is configured by a material dependent 3×3 matrix $\mathbf{\Lambda}$ as $\sigma^\mu \Lambda_\mu^\nu p_\nu$. The properties of the interface subgap states depend on the relative choices of $\mathbf{\Lambda}$ in the two TIs. Generally speaking, $\mathbf{\Lambda}$ in one TI is transformable to $\mathbf{\Lambda}$ in the other not only by the inversion but also by the rotation. The former is a discrete transformation but the latter is a continuous one.

In this paper, we discuss the properties of the two-dimensional states appearing at the interface of two three-dimensional TIs which have different configuration in the spin-orbit coupling. The configuration of the spin-orbit coupling is mainly characterized by the two transformations: (i) the sign inversion in the spin-orbit coupling term for the momentum perpendicular to the interface plane and (ii) the continuous rotation of

the momentum-spin locking angle (ϕ) within the parallel plane to the interface. In the analytical calculation, we obtain the spectra of the interface subgap states in the presence of both the time-reversal symmetry and band-inversion symmetry. When the two topological insulators have the same sign in the transformation (i), the zero-energy surface states appear only at the unique angle of ϕ in the transformation (ii). The zero-energy states in this case are characterized by the mirror Chern number⁷ and fragile under the continuous transformation (ii). When the two topological insulators have the opposite sign to each other in the transformation (i), on the other hand, the gapless surface state appears for all angles in the transformation (ii). The gapless states for the latter case are protected by the Sato's winding number¹⁴⁻¹⁷ and robust under the the continuous transformation (ii). We also carry out numerical simulation on the three-dimensional tight-binding model to check the robustness of interface states at the zero-energy under the perturbations breaking the time-reversal symmetry or band-inversion symmetry. It has been already known that the surface state of a single TI are sensitive to the direction of Zeeman field¹⁸⁻²¹. We find that the interface states at the zero-energy are also sensitive to the direction of Zeeman field. In the presence of the Zeeman field parallel to the interface plane, the zero-energy interface states protected by the mirror Chern number vanish, whereas those protected by the Sato's winding number remain unchanged. In the presence of the Zeeman field perpendicular to the interface plane, on the other hand, the zero-energy interface states protected by the mirror Chern number remain unchanged, whereas those protected by the Sato's winding number vanish. The perturbations breaking the band inversion symmetry remove the interface zero-energy state in both cases.

This paper is organized as follows. In Sec. II, we explain the theoretical model considered in this paper. The analytical expression for the spectra of the interface states is given. In Sec. III, we discuss analytical results of the interface states for two types of junctions. At the same time, we check the robustness of the zero-energy

interface states by the numerical simulation on the tight-binding model. The conclusion is given in Sec. IV.

II. MODEL

The most simple Hamiltonian of three-dimensional topological insulator reads,

$$H_{\text{TI}} = \begin{pmatrix} (m - b\mathbf{p}^2)\sigma^0 & a\boldsymbol{\sigma} \cdot \mathbf{p} \\ a\boldsymbol{\sigma} \cdot \mathbf{p} & -(m - b\mathbf{p}^2)\sigma^0 \end{pmatrix}, \quad (1)$$

where a , b , and m are positive constants, $M = (m - b\mathbf{p}^2)$, σ^0 is 2×2 identity matrix, and $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ are Pauli matrices in spin space. The eigen values of the Hamiltonian are $\pm E_p$ with $E_p = \sqrt{M^2 + a^2|\mathbf{p}|^2}$. For convenience, we utilize the short notation as,

$$H_{\text{TI}} = a\alpha^\mu p_\mu + M\beta, \quad \mu = x, y, z \quad (2)$$

where M is regarded as the Dirac mass and we use 4×4 Dirac matrices,

$$\alpha^\mu = \begin{pmatrix} 0 & \sigma^\mu \\ \sigma^\mu & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} \sigma^0 & 0 \\ 0 & -\sigma^0 \end{pmatrix}.$$

Eq. (2) is called Dirac Hamiltonian and describes topological materials such as topological superconductors and superfluid $^3\text{He-B}$ phase^{22–24}. In real topological insulators, the coupling between spin and orbital parts has more general form

$$H_0 = a\alpha^\mu \Lambda_\mu^\nu p_\nu + M\beta, \quad (3)$$

where the configuration matrix Λ_μ^ν defines the angle which locks spins and momenta and describes the rotation or the inversion in momentum space. In such case, Λ_μ^ν is the real symmetric matrix satisfying $\Lambda_\mu^\nu \Lambda_\mu^\lambda = \delta_\lambda^\nu$. The Z_2 topological number does not distinct two topological insulators with different Λ_μ^ν because they are connected with each other by a unitary transformation²⁵. Thus the energy spectra of Eq. (3) are independent of Λ_μ^ν .

When we focus only on a isolated topological insulator, physics of of Eq. (2) is the same as that of the simple Hamiltonian in Eq. (2). However, when we consider a junction of two different topological insulators, physics happening near the junction interface depends on the choice of Λ_μ^ν in the two topological insulators. This is because there is no unitary transformation which transforms the two different Λ_μ^ν into the Hamiltonian in Eq. 3 at the same time. In the following, we study the properties of subgap states at the junction interface of two different topological insulators. We apply two theoretical methods to analyse the spectra of the interface states. At first, we analytically derive the energy spectra of the interface states from the boundary condition of wave functions. This method gives analytical expression of the subgap spectra of the interface states. Its applicability,

however, is limited to the Hamiltonian preserving of the band-inversion and the time-reversal symmetry. In addition to the analytical method, we also perform numerical simulation on the three-dimensional tight-binding model to check the robustness of the predicted gapless states by the analytic method. They are complementary methods with each other and gives the consistent results.

A. Spectra of interfacial bound states

We begin with the Hamiltonian in Eq. (3) which is represented as

$$H_0 = \begin{bmatrix} M\sigma^0 & a\sigma^\nu \Lambda_\nu^\lambda p_\lambda \\ a\sigma^\nu \Lambda_\nu^\lambda p_\lambda & -M\sigma^0 \end{bmatrix}. \quad (4)$$

The Hamiltonian in Eq. (4) preserves the band-inversion symmetry.

$$\mathcal{D}H(\mathbf{p})\mathcal{D}^{-1} = -H^*(-\mathbf{p}), \quad (5)$$

$$\mathcal{D} = \begin{pmatrix} 0 & -\sigma^y \\ \sigma^y & 0 \end{pmatrix}. \quad (6)$$

The wave function can be given by

$$\Psi_{\mathbf{p}}^{(+)}(\mathbf{r}) = \begin{bmatrix} u_p \sigma^0 \\ v_p \Gamma \end{bmatrix} e^{i\mathbf{p} \cdot \mathbf{r}}, \quad \Psi_{\mathbf{p}}^{(-)}(\mathbf{r}) = \begin{bmatrix} -v_p \Gamma \\ u_p \sigma^0 \end{bmatrix} e^{i\mathbf{p} \cdot \mathbf{r}}, \quad (7)$$

$$\Gamma = \frac{\sigma^\nu \Lambda_\nu^\lambda p_\lambda}{|\mathbf{p}|}, \quad E_p = \sqrt{M^2 + a^2|\mathbf{p}|^2} \quad (8)$$

$$u_p = \sqrt{\frac{1}{2} \left(1 + \frac{M}{E_p} \right)}, \quad v_p = \sqrt{\frac{1}{2} \left(1 - \frac{M}{E_p} \right)}, \quad (9)$$

where $\Psi^{(+)}$ and $\Psi^{(-)}$ are the wave functions belonging to E_p and $-E_p$, respectively. It is evident that E_p is independent of Λ_μ^ν .

When two topological insulators touch with each other at $z = 0$, the wave function for $E = E_p > 0$ are represented by

$$\Psi^{(1)}(\mathbf{r}) = \left[\begin{pmatrix} v\sigma^0 \\ u\Gamma_{(1)}^- \end{pmatrix} e^{-ik_z^+ z} \hat{A} + \begin{pmatrix} u\sigma^0 \\ v\Gamma_{(1)}^+ \end{pmatrix} e^{ik_z^- z} \hat{B} \right] \times e^{i\mathbf{k} \cdot \boldsymbol{\rho}}, \quad (10)$$

for $z < 0$ and

$$\Psi^{(2)}(\mathbf{r}) = \left[\begin{pmatrix} u\sigma^0 \\ v\Gamma_{(2)}^- \end{pmatrix} e^{-ik_z^- z} \hat{C} + \begin{pmatrix} v\sigma^0 \\ u\Gamma_{(2)}^+ \end{pmatrix} e^{ik_z^+ z} \hat{D} \right] \times e^{i\mathbf{k} \cdot \boldsymbol{\rho}}, \quad (11)$$

for $z > 0$ with

$$\Gamma_{(l)}^\pm = \frac{1}{|\mathbf{p}|} \sigma^\nu (\Lambda_{(l)})_\nu^\lambda (p_\pm)_\lambda, \quad \mathbf{p}_\pm = (\mathbf{k}, \pm k_z), \quad (12)$$

$$u = \sqrt{\frac{1}{2} \left(1 + \frac{\Omega}{E} \right)}, \quad v = \sqrt{\frac{1}{2} \left(1 - \frac{\Omega}{E} \right)}, \quad (13)$$

$$\Omega = \sqrt{E^2 - E_g^2}, \quad k_z^\pm = k_0 \sqrt{1 \pm \frac{\Omega}{bk_0^2}}, \quad (14)$$

$$\mathbf{p} = (\mathbf{k}, k_z), \quad \mathbf{k} = (k_x, k_y), \quad \boldsymbol{\rho} = (x, y), \quad (15)$$

$$p_F = \sqrt{\frac{m}{b} - \frac{a^2}{2b^2}}, \quad k_0 = \sqrt{p_F^2 - |\mathbf{k}|^2}, \quad (16)$$

$$E_g = a \sqrt{\frac{m}{b} - \frac{a^2}{4b^2}}, \quad (17)$$

where $l = 1$ and 2 indicate the two topological insulators. The 2×1 coefficient matrices \hat{A} , \hat{B} , \hat{C} , and \hat{D} represent the amplitude of outgoing waves from the interface. At a surface of a topological insulator, it is easy to confirm that the spectra of the surface state become $E = a|\mathbf{k}|$ from the boundary condition $\Psi^{(1)}(\mathbf{r})|_{z=0} = 0$.

At the interface of the two topological insulators, the boundary conditions at $z = 0$,

$$\Psi^{(1)}(\boldsymbol{\rho}, 0) = \Psi^{(2)}(\boldsymbol{\rho}, 0), \quad (18)$$

$$\partial_z \Psi^{(1)}(\boldsymbol{\rho}, z)|_{z=0} = \partial_z \Psi^{(2)}(\boldsymbol{\rho}, z)|_{z=0}, \quad (19)$$

gives a condition

$$\begin{aligned} & \det \left[(k_z^+ - k_z^-)^2 u^2 v^2 \left(\Gamma_{(2)}^+ - \Gamma_{(1)}^- \right) \left(\Gamma_{(2)}^- - \Gamma_{(1)}^+ \right) \right. \\ & \left. - 4k_z^+ k_z^- \left(u^2 \Gamma_{(1)}^- - v^2 \Gamma_{(2)}^- \right) \left(u^2 \Gamma_{(2)}^+ - v^2 \Gamma_{(1)}^+ \right) \right] = 0. \end{aligned} \quad (20)$$

In the quasiclassical approximation, we use a relation $a^2 \ll mb$, which allows $|k_z^+ - k_z^-|^2 \ll k_z^+ k_z^- \approx k_0^2$. Thus we find

$$\det \left[u^2 \Gamma_{(1)}^- - v^2 \Gamma_{(2)}^- \right] \det \left[u^2 \Gamma_{(2)}^+ - v^2 \Gamma_{(1)}^+ \right] = 0. \quad (21)$$

From the condition, we obtain the energy of interface subgap states

$$E = ap_F \sqrt{\frac{|\mathbf{p}|^2 + (p_{\pm})^\nu \left[\Lambda_{(1)} \Lambda_{(2)}^{-1} \right]_\nu^\lambda (p_{\pm})_\lambda}{2|\mathbf{p}|^2}}. \quad (22)$$

The results indicate the spectra of subgap interface states depend on relative choice of $\Lambda_{(1)}$ and $\Lambda_{(2)}$. Within Eq. (4), the spectra obtained from Eq. (21) shown in Eq. (22) always doubly degenerate.

B. Numerical simulation on tight-binding model

To confirm obtained results in the analytical method and to check the robustness of the interface gapless states under perturbations, we also perform the numerical calculation on the tight-binding model. We describe the topological insulator by using the two-band model as

$$H_0(\mathbf{k}; j, j') = \begin{bmatrix} M\sigma^0 & h_{so} \\ h_{so} & M\sigma^0 \end{bmatrix}, \quad (23)$$

$$M = (m + 2b_2(\cos(k_x c_0) + \cos(k_y c_0)) - 2)\delta_{j,j'} - 2b_1\delta_{j,j'} + b_1(\delta_{j,j'+1} + \delta_{j,j'-1}), \quad (24)$$

$$h_{so} = a_2\sigma^\nu [\Lambda_\nu^x \sin(k_x c_0) + \Lambda_\nu^y \sin(k_y c_0)] \delta_{j,j'} - ia_1\sigma^\nu \Lambda_\nu^z (\delta_{j,j'+1} - \delta_{j,j'-1}), \quad (25)$$

where $\mathbf{k} = (k_x, k_y)$, and j represents the place in the z -direction. We apply the periodic boundary condition in the xy -plane and the hard wall boundary condition in the z -axis. We choose $a_1 = 7.86m/c_0$, $a_2 = 14.6m/c_0$, $b_1 = 3.57 \times 10m/c_0^2$, $b_2 = 2.02 \times 10^2 m/c_0^2$ with the lattice constant c_0 being 5 [\AA] in both sides taking into account band structures of Bi_2Se_3 ²⁶. In the simulation, the length of the each topological insulator in the z -direction is $400 c_0$.

To check the robustness of the interfacial zero-energy states, we also consider two types of perturbations in addition to Eq. (23)

$$H_{\text{BI}}(j, j') = 1_{4 \times 4} \times \begin{cases} \mu_{(1)}\delta_{j,j'} + b_{(1)}(\delta_{j,j'+1} + \delta_{j,j'-1}) & \text{for } j < 0 \\ \mu_{(2)}\delta_{j,j'} + b_{(2)}(\delta_{j,j'+1} + \delta_{j,j'-1}) & \text{for } j > 0 \end{cases} \quad (26)$$

$$H_{\text{TR}} = \begin{bmatrix} \mathbf{h} \cdot \boldsymbol{\sigma} & 0 \\ 0 & \mathbf{h} \cdot \boldsymbol{\sigma} \end{bmatrix}. \quad (27)$$

Eq. (26) represents the constant shift of the chemical potential and the band asymmetry in the two TI which break the band-inversion symmetry. Eq. (27) represents the uniform Zeeman potential which breaks the time-reversal symmetry.

III. RESULTS

In what follows, we fix $\Lambda_{(2)}$ at $\text{diag}(1,1,1)$ and study the spectra of the interface for several choices of $\Lambda_{(1)}$ because the relative configuration of momentum-spin locking is responsible for this physics.

A. Rotation within the xy -plane

When we choose

$$\Lambda_{(1)} = \begin{bmatrix} \cos \phi & -\sin \phi & 0 \\ \sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad (28)$$

the spectra in Eq. (22) become

$$E = a \sqrt{p_F^2 - |\mathbf{k}|^2 \sin^2(\phi/2)}. \quad (29)$$

The spin-orbit interaction in Eq. (28) describes only the continuous rotation of spin-momenta locking angle ϕ within the xy plane. The spin-momenta locking in the z axis is common in the two topological insulators. In the effective model around the Γ point in the Brillouin zone, the zero-energy state is possible only at $|\mathbf{k}| = p_F$ and $\theta = \pi$. In Fig. 1, we show numerical results of the dispersion relations for several choices of continuous transformation of ϕ . The dispersions are plotted as a function of k_x because the numerical results are totally isotropic in momentum space. It is evident that the interface subgap state is absent at $\phi = 0$ because the resulting relation

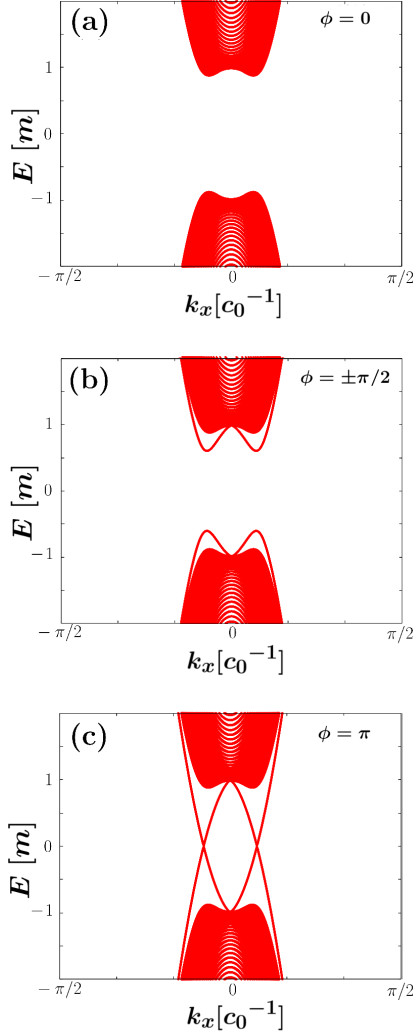


FIG. 1. The energy dispersion of interface states along k_x is shown for Eq. (28). The dispersion has the rotational symmetry in two-dimensional momentum. We choose $\phi = 0, \pi/2$, and π in (a), (b), and (c), respectively. In agreement with the expression in Eq. (29), the zero-energy states appear only $\phi = \pi$ as shown in (c).

$\Lambda_{(2)} = \Lambda_{(1)}$ means the junction of two identical topological insulators. The gap of the interface state decreases with increasing ϕ to π as shown in Figs. 1(a) and 1(b). The wave numbers at the minima in the upper band and the maxima in the lower band have the ring-shaped in two dimensional Brillouin zone. At $\phi = \pi$, such minima and maxima are touched with each other as shown in Fig. 1(c). The surface state becomes gapless and has ring-shaped Fermi surface. The dispersion along radial momentum represent a linear dispersion from the ring-shaped zeros. Such ring-shaped zeros have been discussed in Ref. 7. The choice of $\phi = \pi$ corresponds to the inversion of the two axes within the interface plane, which results in the opposite helicities in the two topological insulators. A topological number derived from the Mirror symmetry

distinguishes the two topological insulators and protects the zero-energy state⁷. However, our numerical calculation suggests that the gapless state appears only at $\phi = \pi$. Therefore the delicate material tuning is necessary for having the ring-shaped zero-energy state. A small perturbation modifying the locking angle ϕ and may open the gap. In fact, Takahashi et al.⁷ has tried to find reasonable combinations of two different topological insulators such as Bi_2Se_3 , Bi_2Te_3 , and Sb_2Te_3 .

Next we check the robustness of the gapless interface state at $\phi = \pi$ by introducing the Zeeman effect in Eq. (27) which breaks time reversal symmetry. In

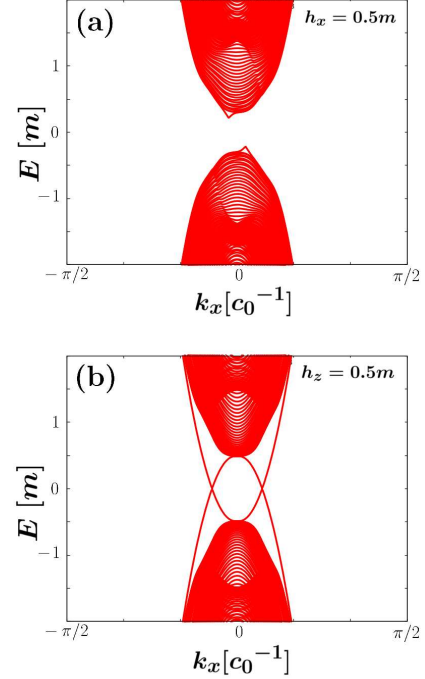


FIG. 2. The energy dispersion of interface states along k_x under the Zeeman field are shown for Eq. (28) with $\phi = \pi$. The figure (a) and (b) are calculated in the presence of the Zeeman field of $h_x = 0.5m$ and $h_z = 0.5m$, respectively.

Fig. 2(a), we consider the Zeeman field parallel to the interface plane with $h_x = 0.5m$ and $h_y = h_z = 0$. The interface state between the two topological insulators becomes gapped in the presence of the in-plane Zeeman field. The Zeeman field perpendicular to the xy -plane, on the other hand, does not remove the gapless interface state shown in Fig. 2(b), where $h_z = 0.5m$ and $h_x = h_y = 0$. Thus the robustness of the interface zero-energy state depends on the direction of the Zeeman field. We note that the tendency in the magnetic anisotropic effect of the interface states is opposite to that found in the gapless surface state of a single topological insulator^{21,27}. This discrepancy, however, is not surprising at all. The helicity is defined in terms of the spin-orbit coupling including the in-plane momenta in Eq. (3). Thus the perpendicular Zeeman field does not affect the spin-

orbit coupling between parallel momenta and spin.

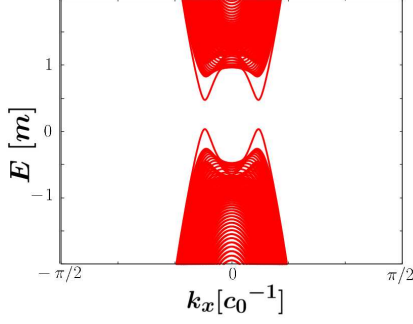


FIG. 3. The energy dispersion of interface states along k_x with magnetization is shown for Eq. (28) with $\phi = \pi$. The figure are calculated in the presence of the band asymmetry as $\mu_{(1)} = -\mu_{(2)} = 0.1m$ and $b_{(1)} = 0.1b_1$.

In Fig. 3(a), we calculate the energy dispersion at $\phi = \pi$ in the presence of the band asymmetry in Eq. (26), where we introduce $\mu_{(1)} = -\mu_{(2)} = 0.1m$, $b_{(1)} = 0.1b_1$ and $b_{(2)} = 0$ in Eq. (4). Obviously, the band asymmetry removes the gapless interface state. Therefore, it would be difficult to find the gapless state at $\phi = \pi$ in Eq. (28) in realistic junctions.

B. Inversion of the z -axis

Next we choose

$$\Lambda_{(1)} = \begin{bmatrix} \cos \phi & -\sin \phi & 0 \\ \sin \phi & \cos \phi & 0 \\ 0 & 0 & -1 \end{bmatrix}. \quad (30)$$

The spin-orbit interaction in Eq. (30) describes the inversion in the z axis plus the continuous rotation of spin-momenta locking angle ϕ within the xy plane. The inversion of the z axis cannot be described by the continuous transformation. The spectra in Eq. (22) becomes

$$E = a|\mathbf{k}| |\cos(\phi/2)|. \quad (31)$$

At $\phi \neq \pi$, the interface state is described by the Dirac cone with the Dirac node at $\mathbf{k} = 0$. We note that this conclusion holds for all ϕ . Thus realizing the Dirac cone like interface gapless state in Eq. (30) is rather easier than that of the ring-shaped zeros in Eq. (28) with $\phi = \pi$.

At $\mathbf{k} = 0$, Eq. (4) is block diagonal for each spin space. It is possible to define the Sato's one-dimensional winding number in each spin sector^{14–16}. Details are shown in Appendix. By using the winding number defined in each spin sector, it is possible to topologically distinct the two topological insulators. The topological numbers are calculated as

$$\mathcal{W}_{(1),\uparrow} = -1, \quad \mathcal{W}_{(1),\downarrow} = 1 \quad (32)$$

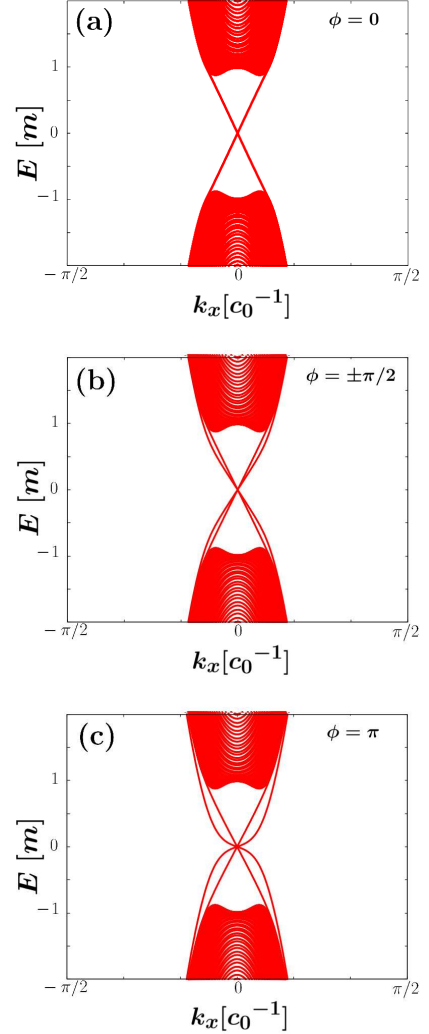


FIG. 4. The energy dispersion of interface states along k_x is shown for Eq. (30). We choose $\phi = 0, \pi/2$, and π in (a), (b), and (c), respectively. The gapless interface state appears for all ϕ , which shows the robustness of the gapless state against the changing the rotation angle ϕ .

for $z < 0$ and

$$\mathcal{W}_{(2),\uparrow} = 1, \quad \mathcal{W}_{(2),\downarrow} = -1 \quad (33)$$

for $z > 0$. The bulk-boundary correspondence suggests the number of zero-energy states for spin-up space is equal to $|\mathcal{W}_{(1),\uparrow} - \mathcal{W}_{(2),\uparrow}| = 2$ and that for spin-down one is $|\mathcal{W}_{(1),\downarrow} - \mathcal{W}_{(2),\downarrow}| = 2$. As a consequence, four states are degenerate at the zero-energy and at $\mathbf{k} = 0$.

The analytical results are confirmed by numerical calculation in Fig. 4, where we plot the dispersions as a function of k_x for Eq. (30) with $\phi = 0, \pi/2$ and π . The numerical results in Fig. 4(a) show the doubly degenerate Dirac cones at the interface in argument with the analytical results. In Fig. 4(b), the numerical results deviate from the analytical one and the two Dirac cones separate from each other as $|k_x|$ increases from zero. The ana-

lytical results in Eq. (31) indicate the flat zero-energy interface states at $\phi = \pi$ for all \mathbf{k} . However, the quasiclassical approximation is not valid at $\phi = \pi$. In fact, the two determinants of matrices in Eq. (21) are automatically proportional to E^2 at $\phi = \pi$. In such case, we need to analyse more general condition in Eq. (20) beyond the quasiclassical approximation. The numerical results in Fig. 2(c) also show the existence of four zero-energy state at $\phi = \pi$. One of the branch shows the linear dispersion, whereas the other seems to have the quadratic dispersion from $\mathbf{k} = 0$ as shown in Fig. 4(c). We note that the choice of $\phi = \pi$ corresponds to the inversion in all axes.

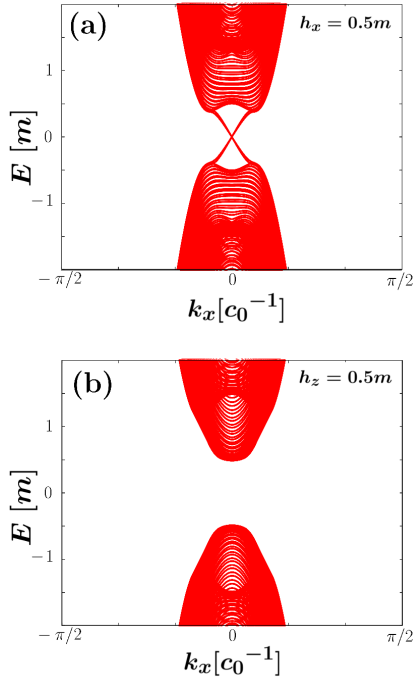


FIG. 5. The energy dispersion of interface states along k_x with magnetization is shown for Eq. (30) at $\phi = 0$. The figure (a) and (b) are calculated in the presence of Zeeman field in the xy plane $h_x = 0.5m$ and that in the perpendicular to the xy plane $h_z = 0.5m$, respectively.

We check the robustness of the zero-energy states under the perturbations breaking the time reversal symmetry in Eq. (27). In Fig. 5(a) and (b), we show the dispersion of the interface states in the presence of the Zeeman fields within the xy plane with $h_x = 0.5m, h_y = 0$ and $h_z = 0$ in (a) and the Zeeman field perpendicular to the xy plane with $h_x = h_y = 0$ and $h_z = 0.5m$ in (b). The results in Fig. 5(a) show that the two Dirac nodes stay at the zero-energy and at $\mathbf{k} = 0$ in the Brillouin zone even in the in-plane Zeeman field. The Sato's number cannot be well defined any longer in the absence of the time-reversal symmetry. However, the zero-energy states under Eq. (30) are very robust even in the in-plane Zeeman field. When we apply the Zeeman field along the z -axis, on the other hand, the interface zero-energy states

vanish as shown in Fig. 5(b). Therefore the robustness of the zero-energy states also depends on the direction of the Zeeman field. The zero-energy states are sensitive (insensitive) to the Zeeman field in the perpendicular (parallel) Zeeman field to the xy plane, which is the opposite tendency to that in Fig. 2(a) and (b). But such tendency is consistent with that found in the topological gapless states at the surface of $^3\text{He-B}$ phase²⁸⁻³⁰. Indeed, by the unitary transformation, Eq. (4) is deformed into

$$U_{\text{TH}} = \begin{bmatrix} 0 & 1 \\ -i\sigma^y & 0 \end{bmatrix}, \quad (34)$$

$$U_{\text{TH}} h_0 U_{\text{TH}}^\dagger = \begin{bmatrix} -M\sigma^0 & a\boldsymbol{\sigma} \cdot \mathbf{p} i\sigma^y \\ -i\sigma^y a\boldsymbol{\sigma} \cdot \mathbf{p} & M\sigma^0 \end{bmatrix}. \quad (35)$$

The last Hamiltonian is nothing other than the Hamiltonian of $^3\text{He-B}$ phase²⁴. The surface Majorana state of $^3\text{He-B}$ phase is protected not only by Z_2 number but also by the Sato's one. The common magnetic anisotropy found in the two systems might be originated from the same topological nature of the wave function.

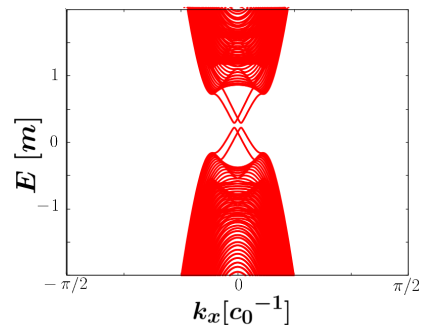


FIG. 6. The energy dispersion of interface states along k_x is shown for Eq. (30) at $\phi = 0$. The results are calculated in the presence of chemical potentials of $\mu_{(1)} = -\mu_{(2)} = 0.2m$ and the band asymmetry $b_{(1)} = 0.1b_1$ and $b_{(2)} = 0$.

In Fig. 6, we discuss effects of the perturbation breaking the band-inversion symmetry in Eq. (26) with $\mu_{(1)} = -\mu_{(2)} = -0.2m$, $b_{(1)} = 0.1b_1$ and $b_{(2)} = 0$. The two Dirac cones are lifted off from each other and the gap is opening in the absence of the band-inversion symmetry. The Sato's number cannot be defined in the absence of the band inversion symmetry. Therefore there is no reason for the interface states remaining gapless.

C. Remaining configurations

Finally we choose

$$\Lambda_{(1)} = \begin{bmatrix} s & 0 & 0 \\ 0 & \cos \phi & -\sin \phi \\ 0 & \sin \phi & \cos \phi \end{bmatrix}, \quad (36)$$

with $s = \pm 1$. For $s = 1$, the transformation represents only the continuous rotation within yz -plane. The gapless states appear only at $\phi = \pi$. Because x and y axes

are no longer equivalent to each other, the dispersion becomes anisotropic in the two-dimensional Brillouin zone as shown in Figs. 7(a) and 7(b). Here we plot the dispersion as a function of k_x at $k_y = 0$ in Fig. 7(a). The results suggest the doubly degenerate Dirac cones. On the other hand, Fig. 7(a) shows the dispersion along k_y at $k_x = 0$. The two dispersion branches clearly separate from each other. The Dirac nodes, however, stay at $\mathbf{k} = 0$.

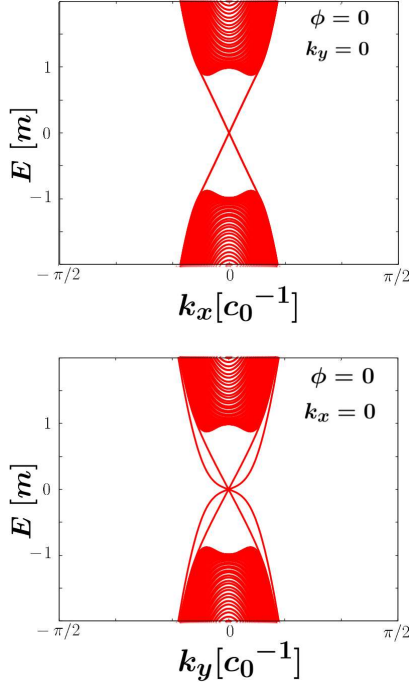


FIG. 7. The energy dispersion of interface states in Eq. (36) with $s = 1$ and $\phi = \pi$. In (a), k_y is fixed at the origin and the energy is plotted as a function of k_x . In (b), k_x is fixed at the origin and the energy is plotted as a function of k_y .

When we choose $s = -1$, Eq. (36) represents the inversion in the x axis. The choice of $\phi = \pi$ in Eq. (36) is identical to Eq. (30) with $\phi = \pi$ whose results are shown in Fig. 4(c). Therefore we seek gapless states for $\phi \neq \pi$. The results for $\phi = 0$ are shown in Figs. 8(a) and 8(b). We plot the dispersion as a function of k_x at $k_y = 0$ in Figs. 8(a). The results suggest that there are the two Dirac cones but their nodes stay at finite value of k_x . Correspondingly, there is gapless state in the dispersion along the k_y at the Dirac point of $k_x = k_D = 0.094\pi$ in Fig. 8(b). The similar dispersion can be seen also at $\phi = \pm\pi/2$ as shown in Fig. 8(c). At $s = -1$, Eq. (36) includes the inversion in x direction. In such case, two Dirac cones appear with their nodes staying on k_x axis and these cones come close to the origin of $\mathbf{k} = 0$ as increasing of ϕ to π in Fig. 4(c).

The rotation in xz -plane is equivalent to that in yz -plane under interchanging k_x and k_y . Thus the Dirac nodes are stay on the k_y axis when we consider inversion in the y direction. Together with the results in Fig. 4(c),

we conclude that the gapless states appear when the relative configuration matrix $\Lambda_{(1)}$ includes the inversion in odd number axes. Unfortunately, these gapless states are also fragile under the perturbation which breaks the-band inversion symmetry.

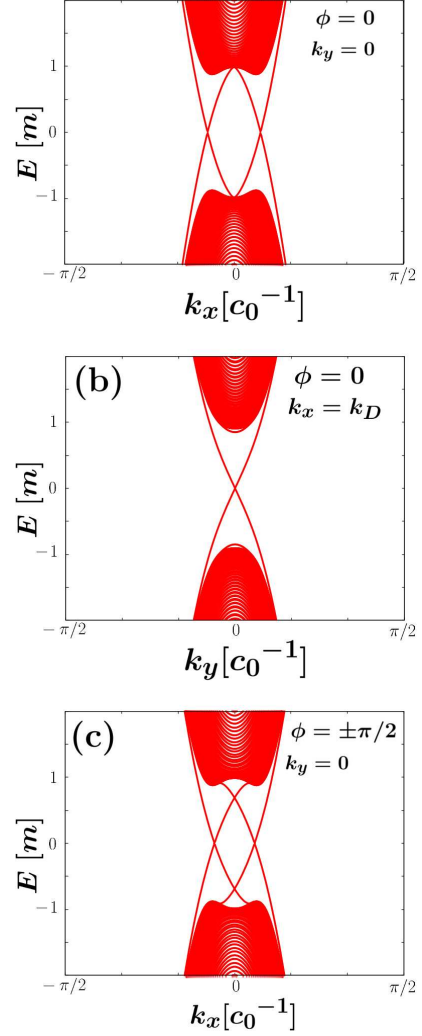


FIG. 8. The energy dispersion of interface states along (a) k_x and (b) k_y are shown at $\phi = 0$ and $s = -1$. In the figure (b), we set k_x at the Dirac point $k_D = 0.094\pi$. The figure (c) is energy dispersion along k_x at $\phi = \pi/2$ and $s = 1$.

IV. CONCLUSION

We have studied the interface state between two topological insulators with different configurations of spin-orbit interactions. The two topological insulators are touching at $z = 0$ and its interface is flat within the xy plane. The coupling of spin σ with momenta \mathbf{p} is configured by a material dependent 3×3 matrix Λ as $\sigma^\mu \Lambda_\mu^\nu p_\nu$. The spectra of subgap states depends on relative configuration matrix $\Lambda_{(1)} = \Lambda_{(1)} \Lambda_{(2)}^{-1}$, where $\Lambda_{(l)}$ for $l = 1$ and

2 characterize the spin-orbit coupling in the two topological insulators. The properties of interface gapless states in the presence of the time-reversal symmetry and the band-inversion symmetry are summarized as follows.

(i) When Λ_{12} includes the inversion along one-axis, two Dirac cones appears in the two-dimensional Brillouin zone. When the inversion axis is in z direction, the doubly degenerate Dirac cones appear and their nodes stay at the Γ -point ($k_x = k_y = 0$). When the inversion axis is in x (y) direction, the two Dirac cones are separated in the Brillouin zone and their nodes stay on x (y) axis. In this case, the Dirac nodes are robust even if Λ_{12} includes the rotation around the inversion axis.

(ii) When Λ_{12} includes the inversion in two-axes, the spectra depends also on the choices of the two-axes. When the two-axes are x and y , the junction have the mirror symmetry and the ring-shaped zeros appear in the Brillouin zone. When one of the two-axes is z and the other is x (y), two Dirac nodes appear at the Γ -point. The dispersion of them are degenerate along k_y (k_x) but the degeneracy is lifted along k_x (k_y). In this case, the Dirac nodes are fragile under the rotation Λ_{12} around any axis.

(iii) When Λ_{12} includes the inversion in all axes, non-degenerate two Dirac cones appear and their nodes stay at the Γ -point. This situation can be regarded as the series transformation of (i) and (ii). Therefore, the robust gapless state against rotation of ϕ is realised under the inversion in odd number of axes.

The numerical results show that the interface gapless states are sensitive to the direction of the Zeeman field breaking the time-reversal symmetry. They are robust under the Zeeman field in one direction, but fragile under the Zeeman field in another direction. Unfortunately, all gapless states are fragile in the presence of the perturbations breaking the band-inversion symmetry. The last property implies the difficulty of finding the gapless states within the combination of existing topological insulators. However, our results predict unusual gapless state appearing at the interface of two different topological superconductors and that of two different superfluid phases. This is because Bogoliubov-de Gennes Hamiltonian similar to Eq. (3) always satisfies the particle-hole symmetry (band-inversion symmetry in this paper) so called as chiral symmetry in Ref. 24.

V. ACKNOWLEDGMENTS

The authors are grateful to M. Sato for useful discussion. This work was supported by the "Topological

Quantum Phenomena" (No. 22103002) Grant-in Aid for Scientific Research on Innovative Areas from the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan.

Note - In the very final stages of preparation of this manuscript, we have been made aware of another work which has some overlap with ours: Ref. [31]

Appendix A: Sato's winding number

When we choose

$$\Lambda = \begin{bmatrix} \cos \phi & -\sin \phi & 0 \\ \sin \phi & \cos \phi & 0 \\ 0 & 0 & s \end{bmatrix}, \quad (\text{A1})$$

with $s = \pm 1$, the Hamiltonian in Eq. (4) at $\mathbf{k} = 0$ is block diagonal in each spin space irrespective of ϕ . Namely

$$H_{\uparrow} = \begin{bmatrix} M_z & ask_z \\ ask_z & -M_z \end{bmatrix}, \quad H_{\downarrow} = \begin{bmatrix} M_z & -ask_z \\ -ask_z & -M_z \end{bmatrix}, \quad (\text{A2})$$

with $M_z = m - bk_z^2$. For instance, eigen values of H_{\uparrow} are $\pm \epsilon_{k_z}$ and eigen vectors are represented by

$$\begin{bmatrix} \cos(\theta_{k_z}/2) \\ \sin(\theta_{k_z}/2) \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} -\sin(\theta_{k_z}/2) \\ \cos(\theta_{k_z}/2) \end{bmatrix}, \quad (\text{A3})$$

for ϵ_{k_z} and $-\epsilon_{k_z}$, respectively. Here we define

$$\epsilon_{k_z} = \sqrt{M_z^2 + (ak_z)^2}, \quad (\text{A4})$$

$$\cos \theta_{k_z} = \frac{M_z}{\epsilon_{k_z}}, \quad \sin \theta_{k_z} = \frac{ak_z}{\epsilon_{k_z}}. \quad (\text{A5})$$

In the presence of the time-reversal symmetry, the eigen vectors can be represented only by real quantities. In the presence of the band-inversion symmetry, the Sato's winding number can be defined at $\mathbf{k} = 0$ as

$$\mathcal{W}(\uparrow, s) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_z \partial_{k_z} \theta_{k_z}. \quad (\text{A6})$$

To estimate the topological number, we use tight-binding representation of the Hamiltonian,

$$M_z = m - bk_z^2 \rightarrow m - 2t(1 - \cos k_z), \quad (\text{A7})$$

$$ak_z \rightarrow a_0 t \sin k_z, \quad (\text{A8})$$

with $t > 0$, $m - 4t < 0$, and $|a_0| \ll 1$ is a dimensionless constant. We find that

$$\mathcal{W}(\uparrow, s) = \text{sgn}(s), \quad \mathcal{W}(\downarrow, s) = -\text{sgn}(s). \quad (\text{A9})$$

¹ L. Fu, C. L. Kane, and E. J. Mele, Phys. Rev. Lett. **98**, 106803 (2007).

² L. Fu and C. L. Kane, Phys. Rev. B. **76**, 045302 (2007).

³ J. E. Moore and L. Balents, Phys. Rev. B. **75**, 121306 (2007).

- ⁴ Y. L. Chen, J. G. Analytis, J.-H. Chu, Z. K. Liu, S. K. Mo, X. L. Qi, H. J. Zhang, D. H. Lu, X. Dai, Z. Fang, S. C. Zhang, I. R. Fisher, Z. Hussain, and Z. X. Shen, *Science* **325**, 178 (2009).
- ⁵ P. Roushan, J. Seo, C. V. Parker, Y. S. Hor, D. Hsieh, D. Qian, A. Richardella, M. Z. Hasan, R. J. Cava, and A. Yazdani, *Nature* **460**, 1106 (2009).
- ⁶ T. Zhang, P. Cheng, X. Chen, J.-F. Jia, X. Ma, K. He, L. Wang, H. Zhang, X. Dai, Z. Fang, X. Xie, and Q.-K. Xue, *Phys. Rev. Lett.* **103**, 266803 (2009).
- ⁷ R. Takahashi and S. Murakami, *Phys. Rev. Lett.* **107**, 166805 (2011).
- ⁸ D. Sen and O. Deb, *Phys. Rev. B* **85**, 245402 (2012).
- ⁹ Y. Asano, Y. Tanaka, and N. Nagaosa, *Phys. Rev. Lett.* **105**, 056402 (2010).
- ¹⁰ Y. S. Barash, A. M. Bobkov, and M. Fogelstrom, *Phys. Rev. B* **64**, 214503 (2001).
- ¹¹ H. K. Kwon, *Eur. Phys. J. B* **37**, 349 (2004).
- ¹² J. C. Y. Teo, L. Fu, and C. L. Kane, *Phys. Rev. B* **78**, 045426 (2008).
- ¹³ A. Nishide, A. A. Taskin, Y. Takeichi, T. Okuda, A. Kakizaki, T. Hirahara, K. Nakatsuji, F. Komori, Y. Ando, and I. Matsuda, *Phys. Rev. B* **81**, 041309 (2010).
- ¹⁴ M. Sato and S. Fujimoto, *Phys. Rev. Lett.* **105**, 217001 (2010).
- ¹⁵ K. Yada, M. Sato, Y. Tanaka, and T. Yokoyama, *Phys. Rev. B* **83**, 064505 (2011).
- ¹⁶ M. Sato, Y. Tanaka, K. Yada, and T. Yokoyama, *Phys. Rev. B* **83**, 224511 (2011).
- ¹⁷ T. Mizushima, M. Sato, and K. Machida, *Phys. Rev. Lett.* **109**, 165301 (2012).
- ¹⁸ Y. Tanaka, T. Yokoyama, and N. Nagaosa, *Phys. Rev. Lett.* **103**, 107002 (2009).
- ¹⁹ Q. Liu, C.-X. Liu, C. Xu, X.-L. Qi, , and S.-C. Zhang, *Phys. Rev. Lett.* **102**, 156603 (2009).
- ²⁰ L. A. Wray, S.-Y. Xu, Y. Xia, D. Hsieh, A. V. Fedorov, Y. S. Hor, R. J. Cava, A. Bansil, H. Lin, and M. Z. Hasan, *Nat. Phys.* **7**, 32 (2010).
- ²¹ T. Habe and Y. Asano, *Phys. Rev. B* **85**, 195325 (2012).
- ²² R. Balian and N. R. Werthamer, *Phys. Rev.* **131**, 1553 (1963).
- ²³ A. J. Leggett, *Rev. Mod. Phys.* **47**, 331 (1975).
- ²⁴ A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. W. Ludwig, *Phys. Rev. B* **78**, 195125 (2008).
- ²⁵ C.-X. Liu, X.-L. Qi, H. Zhang, X. Dai, Z. Fang, and S.-C. Zhang, *Phys. Rev. B* **82**, 045122 (2010).
- ²⁶ H. Zhang, C. X. Liu, X. L. Qi, X. Dai, Z. Fang, and S. C. Zhang, *Nat. Phys.* **5**, 438 (2009).
- ²⁷ T. Yokoyama, Y. Tanaka, J. Zang, and N. Nagaosa, *Phys. Rev. B* **81**, 121401(R) (2010).
- ²⁸ Y. Nagato, S. Higashitani, and K. Nagai, *J. Phys. Soc. Jpn.* **78**, 123603 (2009).
- ²⁹ S. B. Chung and S.-C. Zhang, *Phys. Rev. Lett* **103**, 235301 (2009).
- ³⁰ S. Murakawa, Y. Wada, Y. Tamura, M. Wasai, M. Saitoh, Y. Aoki, R. Nomura, Y. Okuda, Y. Nagato, M. Yamamoto, S. Higashitani, and K. Nagai, *J. Phys. Soc. Jpn.* **80**, 013602 (2011).
- ³¹ C. De Beule and B. Partoens, arXiv:1302.3359 (unpublished).